

Use of Quantum Sampling to Calculate Mean Values of Observables and Partition Function of a Quantum System

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Abstract

We describe an algorithm for using a quantum computer to calculate mean values of observables and the partition function of a quantum system. Our algorithm includes two sub-algorithms. The first sub-algorithm is for calculating, with polynomial efficiency, certain diagonal matrix elements of an observable. This sub-algorithm is performed on a quantum computer, using quantum phase estimation and tomography. The second sub-algorithm is for sampling a probability distribution. This sub-algorithm is not polynomially efficient. It can be performed either on a classical or a quantum computer, but a quantum computer can perform it quadratically faster.

1 Introduction

In this paper, we describe an algorithm for using a quantum computer to calculate mean values of observables and the partition function of a quantum system. Our algorithm includes two sub-algorithms.

One sub-algorithm is for calculating, with polynomial efficiency, certain diagonal matrix elements of an observable. This sub-algorithm is performed on a quantum computer, using quantum phase estimation and tomography. This sub-algorithm is very similar to the algorithm of Ref.[1] by Harrow et al., except that we modify it to accomplish a substantially different job that has nothing to do whatsoever with systems of linear equations.

A second sub-algorithm is for sampling a probability distribution. This sub-algorithm is not polynomially efficient. It can be performed either on a classical or a quantum computer. However, a quantum computer can perform it quadratically faster than a classical computer, if one uses a quantum sampling technique based on Szegedy operators, like, for instance, the quantum Gibbs sampling algorithm described in Ref.[2].

We end the paper with a brief section comparing the algorithms proposed in this paper with quantum algorithms proposed in earlier papers for calculating the same things. In particular, we compare our work to Ref.[3] by Wocjan et al., Ref.[4] by Poulin and Wocjan, and Ref.[5] by Temme et al..

2 Location, Location, Location Notation, Notation, Notation

In this section, we will define some notation that is used throughout this paper. For additional information about my notational quirks, I recommend that the reader consult the notation section of some of my previous papers; for example, Ref.[6].

We will often use the symbol N_B for the number (≥ 1) of qubits and $N_S = 2^{N_B}$ for the number of states with N_B qubits. The quantum computing literature often uses n for N_B and N for N_S , but we will avoid this notation. We prefer to use n for the number operator $|1\rangle\langle 1|$.

Let $Bool = \{0, 1\}$. As usual, let $\mathbb{Z}, \mathbb{R}, \mathbb{C}$ represent the set of integers (negative and non-negative), real numbers, and complex numbers, respectively. We will also sometimes add a superscript to the symbols \mathbb{Z}, \mathbb{R} to indicate a subset of these sets. For example, we will use $\mathbb{R}^{\geq 0}$ to denote the non-negative reals. For integers a, b such that $a \leq b$, let $Z_{a,b} = \{a, a+1, \dots, b-1, b\}$.

We will use $\Theta(S)$ to represent the “truth function”; $\Theta(S)$ equals 1 if statement S is true and 0 if S is false. For example, the Kronecker delta function is defined by $\delta_x^y = \delta(x, y) = \Theta(x = y)$.

If $\vec{x} = x_{N_B-1} \dots x_2 x_1 x_0$, where $x_\mu \in Bool$, then $dec(\vec{x}) = \sum_{\mu=0}^{N_B-1} 2^\mu x_\mu = x$.

Conversely, $\vec{x} = \text{bin}(x)$. However, when our meaning is clear from context, we will omit the $\text{bin}()$ and $\text{dec}()$. Hence, in some places x might stand for an element of Z_{0,N_S-1} , and in other places for the corresponding element of Bool^{N_B} .

We won't usually put a caret over a symbol to indicate that it is an operator, but sometimes we will. For example, we will usually use H for a Hamiltonian, but sometimes, for clarity, we will call it \hat{H} .

Note that in our quantum circuit diagrams, time flows from the right to the left of the diagram (this is the **Dirac Convention**). Careful: Many workers in Quantum Computing draw their diagrams so that time flows from left to right (the **Quayle Convention**).

We will say a problem can be solved **with polynomial efficiency**, or **p-efficiently** for short, if its solution can be achieved in a time polynomial in N_B . Here N_B is the number of bits required to encode the input for the algorithm that solves the problem.

By **compiling a unitary matrix**, we mean decomposing it into a **SEO** (Sequence of Elementary Operators), where by elementary operators we mean operators that act on only a few qubits (usually 1, 2 or 3), such as single-qubit rotations and CNOTs. Compilations can be either exact, or approximate (within a certain precision).

We will say a unitary operator U acting on \mathbb{C}^{N_S} can be **compiled with polynomial efficiency**, or **p-compiled** for short, if U can be expressed, either approximately or exactly, as a SEO of length polynomial in N_B . When necessary, we specify whether a p-compilation is exact or approximate.

Next, we explain our notation related to Discrete Fourier Transforms.

For any $x \in Z_{0,N_S-1}$, define k_x by

$$k_x = \frac{2\pi x}{N_S} . \quad (1)$$

Let \hat{k} and \hat{x} be operators acting on \mathbb{C}^{N_S} with eigenvectors and eigenvalues given by

$$\hat{x}|x\rangle = x|x\rangle \quad (2)$$

and

$$\hat{k}|\hat{k} = k_x\rangle = k_x|\hat{k} = k_x\rangle \quad (3)$$

for any $x \in Z_{0,N_S-1}$. Let the eigenvectors of \hat{x} and \hat{k} be related by a ‘‘Discrete Fourier Transformation’’:

$$|\hat{k} = k_x\rangle = \frac{1}{\sqrt{N_S}} \sum_{y=0}^{N_S-1} e^{ik_x y} |y\rangle . \quad (4)$$

Eq.(4) defines a ‘‘basis-changer’’ unitary operator U_{FT} with matrix elements given by

$$\langle y|U_{FT}|x\rangle = \langle y|\hat{k} = k_x\rangle = \frac{1}{\sqrt{N_S}}e^{ik_x y} = \frac{1}{\sqrt{N_S}}e^{ixk_y} . \quad (5)$$

Assume that the eigenstates of \hat{x} are orthonormal and complete:

$$\langle y|x\rangle = \delta(y, x) \quad (6)$$

for all $x, y \in Z_{0, N_S-1}$, and

$$\sum_{x=0}^{N_S-1} |x\rangle\langle x| = 1 . \quad (7)$$

Then it follows that the eigenstates of \hat{k} are orthonormal and complete too, because

$$\langle \hat{k} = k_y|\hat{k} = k_x\rangle = \langle y|U_{FT}^\dagger U_{FT}|x\rangle = \delta(y, x) , \quad (8)$$

and

$$\sum_x |\hat{k} = k_x\rangle\langle \hat{k} = k_x| = \sum_x U_{FT}|x\rangle\langle x|U_{FT}^\dagger = 1 . \quad (9)$$

Often in quantum computing we come across quantum states of the form

$$|\hat{k} = k\rangle = \frac{1}{\sqrt{N_S}} \sum_{y=0}^{N_S-1} e^{iky} |y\rangle , \quad (10)$$

with

$$k = k_z + \Delta k , \quad (11)$$

for some $z \in Z_{0, N_S-2}$ and $0 \leq \Delta k \leq \frac{2\pi}{N_S}$. If k is neither k_z nor k_{z+1} but lies somewhere in between, then $|k\rangle$ is close to but not exactly equal to an eigenstate of \hat{k} . Note that when $\hat{k} = k_z$,

$$\langle x|U_{FT}^\dagger|\hat{k} = k_z\rangle = \langle x|z\rangle = \delta(x, z) . \quad (12)$$

For $\hat{k} = k$ where k is given by Eq.(11), this generalizes to

$$\langle x|U_{FT}^\dagger|\hat{k} = k\rangle = \frac{1}{N_S} \sum_{y=0}^{N_S-1} e^{i(k-k_x)y} \quad (13)$$

$$= \frac{1}{N_S} \frac{1 - e^{i(k-k_x)N_S}}{1 - e^{i(k-k_x)}} \quad (14)$$

$$= \frac{1}{N_S} \frac{e^{i(k-k_x)\frac{N_S}{2}} \sin\left((k-k_x)\frac{N_S}{2}\right)}{e^{i(k-k_x)\frac{1}{2}} \sin\left((k-k_x)\frac{1}{2}\right)} . \quad (15)$$

3 Diagonal Matrix Elements

In this section, we give an algorithm for calculating certain diagonal matrix elements p -efficiently, using a quantum computer. This algorithm will be used as a subroutine in the algorithms proposed in later sections.

The algorithm described in the proof of Claim 1 below is very similar to the algorithm of Ref.[1], except that we modify it to accomplish a different job. In a nutshell, Ref.[1] combines two operations that were separately familiar to most quantum computerists long before Ref.[1]: a phase estimation (PE) operation, followed by a quantum tomography operation.

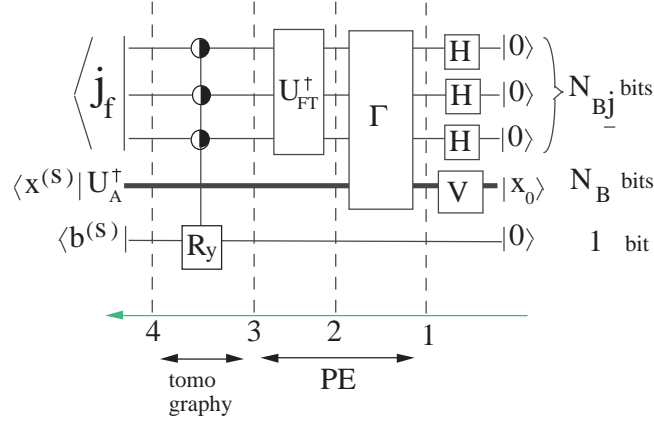


Figure 1: Quantum circuit used in Claim 1 to calculate the diagonal matrix element given by Eq.(16).

Claim 1 *Let A be an N_S dimensional Hermitian matrix with non-negative eigenvalues, V an N_S dimensional unitary matrix, $f : \mathbb{R}^{\geq 0} \rightarrow \mathbb{R}^{\geq 0}$, and $x_0 \in \text{Bool}^{N_B}$, where $N_S = 2^{N_B}$. Assume that f is simple (that is, that it can be calculated p -efficiently). Assume that we know how to p -compile V and $e^{iA\Delta t}$ for any $\Delta t \geq 0$. Then we can calculate p -efficiently the diagonal matrix element*

$$\mu(x_0) = \langle x_0 | V^\dagger f(A) V | x_0 \rangle . \quad (16)$$

proof:

Let $N_{Sj} = 2^{N_{Bj}}$ be the number of states of N_{Bj} bits, for a set of bits labeled j .

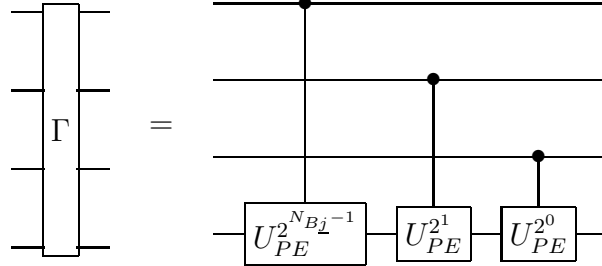
The diagonal matrix element Eq.(16) can be calculated by running on a quantum computer the quantum circuit shown in Fig.1. In that figure, there are three sets of qubits. At the top are N_{Bj} “probe” qubits. Below the probe qubits are the N_B “main” qubits which are initially in state $|x_0\rangle$. Finally, below the main qubits is a single “ancilla” qubit that is used in the final tomography step.

In a moment, we will describe the evolution of the state vector as it courses down this quantum circuit. But before doing so, we need to specify some of the blocks in Fig.1 more precisely.

Note that

$$H^{\otimes N_{B\bar{j}}}|0\rangle^{\otimes N_{B\bar{j}}} = \frac{1}{\sqrt{N_{S\bar{j}}}} \sum_{j=0}^{N_{S\bar{j}}-1} |j\rangle. \quad (17)$$

As for the Γ box, it represents



$$\Gamma = \text{circuit with 4 lines and gates } U_{PE}^{2^{N_{B\bar{j}}-1}}, U_{PE}^{2^1}, U_{PE}^{2^0} \quad (18)$$

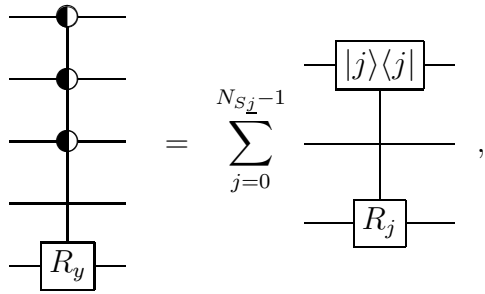


$$= \sum_{j=0}^{N_{S\bar{j}}-1} \text{circuit with } |j\rangle\langle j| \text{ gate on bottom line}, \quad (19)$$

where

$$U_{PE} = e^{iA\Delta t}. \quad (20)$$

(For definiteness, some parts of Eq.(18) assume that $N_{B\bar{j}} = 3$.) Finally, the operation with the “half moon” nodes represents



$$= \sum_{j=0}^{N_{S\bar{j}}-1} \text{circuit with } |j\rangle\langle j| \text{ gate on bottom line}, \quad (21)$$

(note that some parts of Eq.(21) again assume that $N_{B\bar{j}} = 3$.) where R_j is defined by

$$R_j = \begin{bmatrix} c_j & -s_j \\ s_j & c_j \end{bmatrix} \quad (22)$$

with

$$c_j = \sqrt{\gamma f\left(\frac{2\pi j}{\Delta t N_{S_{\underline{j}}}}\right)}, \quad (23)$$

$$s_j = \sqrt{1 - c_j^2}. \quad (24)$$

γ is defined so that $0 \leq c_j \leq 1$ for all $j \in Z_{0, N_{S_{\underline{j}}}-1}$. Eq.(21) is an $SU(2)$ multiplexor with $N_{B_{\underline{j}}}$ controls. It can be p-compiled approximately (the software application “Multiplexor Expander” [7] can do this).

Let

$$A|\hat{A} = A_x\rangle = A_x|\hat{A} = A_x\rangle \quad (25)$$

for $x \in Bool^{N_B}$. Define the basis-changer unitary operator U_A by

$$\langle y|U_A|x\rangle = \langle y|\hat{A} = A_x\rangle \quad (26)$$

for $x, y \in Bool^{N_B}$.

Fig.1 includes at its bottom a time axis marked with notches for times 1 thru 4. Let $|\Psi_t\rangle$ for $t \in Z_{1,4}$ denote the quantum state at those times. Let us represent such states by sums over 3 rows, where the first row refers to the $N_{B_{\underline{j}}}$ probe bits, the second row refers to the N_B main bits, and the final row refers to the single ancilla bit.

One has

$$|\Psi_1\rangle = \begin{bmatrix} \frac{1}{\sqrt{N_{S_{\underline{j}}}}} \sum_{j=0}^{N_{S_{\underline{j}}}-1} |j\rangle \\ \sum_{x=0}^{N_S-1} |\hat{A} = A_x\rangle \langle \hat{A} = A_x|V|x_0\rangle \\ |0\rangle \end{bmatrix}, \quad (27)$$

$$|\Psi_2\rangle = \begin{bmatrix} \sum_{j'=0}^{N_{S_{\underline{j}}}-1} |j'\rangle \langle j'| \frac{1}{\sqrt{N_{S_{\underline{j}}}}} \sum_{j=0}^{N_{S_{\underline{j}}}-1} |j\rangle \\ e^{i\hat{A}\Delta t j'} \sum_{x=0}^{N_S-1} |\hat{A} = A_x\rangle \langle \hat{A} = A_x|V|x_0\rangle \\ |0\rangle \end{bmatrix} \quad (28)$$

$$= \sum_{j=0}^{N_{S_{\underline{j}}}-1} \sum_{x=0}^{N_S-1} \begin{bmatrix} |j\rangle \frac{e^{iA_x\Delta t j}}{\sqrt{N_{S_{\underline{j}}}}} \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x|V|x_0\rangle \\ |0\rangle \end{bmatrix}, \quad (29)$$

$$|\Psi_3\rangle = \sum_{j=0}^{N_{S\bar{j}}-1} \sum_{x=0}^{N_S-1} \left[\begin{array}{l} \sum_{j'=0}^{N_{S\bar{j}}-1} |j'\rangle \langle j'| U_{FT}^\dagger |j\rangle \frac{e^{iA_x \Delta t j}}{\sqrt{N_{S\bar{j}}}} \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x| V |x_0\rangle \\ |0\rangle \end{array} \right] \quad (30)$$

$$= \sum_{x=0}^{N_S-1} \left[\begin{array}{l} \sum_{j'=0}^{N_{S\bar{j}}-1} |j'\rangle \sum_{j=0}^{N_{S\bar{j}}-1} \frac{e^{i(-\frac{2\pi j'}{N_{S\bar{j}}} + A_x \Delta t)j}}{N_{S\bar{j}}} \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x| V |x_0\rangle \\ |0\rangle \end{array} \right] \quad (31)$$

$$= \sum_{x=0}^{N_S-1} \sum_{j'=0}^{N_{S\bar{j}}-1} \left[\begin{array}{l} |j'\rangle \delta(\frac{2\pi j'}{N_{S\bar{j}}}, A_x \Delta t) \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x| V |x_0\rangle \\ |0\rangle \end{array} \right] \quad (32)$$

$$= \sum_{x=0}^{N_S-1} \left[\begin{array}{l} |j = A_x \frac{\Delta t N_{S\bar{j}}}{2\pi}\rangle \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x| V |x_0\rangle \\ |0\rangle \end{array} \right] \quad (33)$$

and

$$|\Psi_4\rangle = \sum_{x=0}^{N_S-1} \left[\begin{array}{l} |j = A_x \frac{\Delta t N_{S\bar{j}}}{2\pi}\rangle \\ |\hat{A} = A_x\rangle \langle \hat{A} = A_x| V |x_0\rangle \\ \sqrt{\gamma f(A_x)} |0\rangle + \sqrt{1 - \gamma f(A_x)} |1\rangle \end{array} \right]. \quad (34)$$

Note that we are treating the quantity $A_x \frac{\Delta t N_{S\bar{j}}}{2\pi}$ as if it were an integer in the range $Z_{0, N_{S\bar{j}}-1}$. This quantity is non-negative because A_x and Δt are non-negative by assumption. Δt can be chosen small enough so that this quantity is always smaller than $N_{S\bar{j}} - 1$. As to whether the quantity is an integer, it need not be in general. When it isn't, one has to do a more careful treatment (as done in Ref.[1]). By using the treatment given above instead of a more careful one like the one of Ref.[1], we are introducing a small error in what we shall say next.

It follows from Eq.(34) that ¹

$$\frac{\langle j_f |}{\langle b^{(s)} |} |\Psi_4\rangle = \delta^{j_f}_{A_{x(s)} \frac{\Delta t N_{S\bar{j}}}{2\pi}} \left[\langle \hat{A} = A_{x(s)} | \sqrt{\gamma f(A)} V |x_0\rangle \delta_{b^{(s)}}^0 + \langle \hat{A} = A_{x(s)} | \sqrt{1 - \gamma f(A)} V |x_0\rangle \delta_{b^{(s)}}^1 \right], \quad (35)$$

¹Note that $\langle \hat{A} = A_{x(s)} | = \langle x^{(s)} | U_A^\dagger$ so if we were actually going to observe the \hat{A} of the main qubits, this would require that we know and apply U_A^\dagger to them and then measure $\langle x^{(s)} |$. However, it turns out that we don't need to observe/measure the main qubits to calculate $\check{P}_{\bar{b}}$, so we don't need to know or apply U_A^\dagger after all.

where $j_f \in Bool^{N_{Bj}}$, $x^{(s)} \in Bool^{N_B}$, $b^{(s)} \in Bool$. The index $s \in Z_{1, N_{sam}}$ labels N_{sam} samples. We can define an empirical probability distribution $\check{P}_{\underline{x}, \underline{b}}$ by

$$\check{P}_{\underline{x}, \underline{b}}(x, b) = \frac{1}{N_{sam}} \sum_{s=1}^{N_{sam}} \delta_x^{x^{(s)}} \delta_b^{b^{(s)}} , \quad (36)$$

where $x \in Z_{0, N_S-1}$ and $b \in Bool$. Then

$$\check{P}_{\underline{x}, \underline{b}}(x, b) \approx \left| \langle \hat{A} = A_x | \sqrt{\gamma f(A)} V | x_0 \rangle \right|^2 \delta_b^0 + \left| \langle \hat{A} = A_x | \sqrt{1 - \gamma f(A)} V | x_0 \rangle \right|^2 \delta_b^1 . \quad (37)$$

Therefore,

$$\check{P}_{\underline{b}}(b) = \sum_{x=0}^{N_S-1} \check{P}_{\underline{x}, \underline{b}}(x, b) = \frac{1}{N_{sam}} \sum_{s=1}^{N_{sam}} \delta_b^{b^{(s)}} , \quad (38)$$

and

$$\check{P}_{\underline{b}}(b) \approx \langle x_0 | V^\dagger \gamma f(A) V | x_0 \rangle \delta_b^0 + \langle x_0 | V^\dagger [1 - \gamma f(A)] V | x_0 \rangle \delta_b^1 . \quad (39)$$

Finally, we conclude that

$$\langle x_0 | V^\dagger f(A) V | x_0 \rangle \approx \frac{\check{P}_{\underline{b}}(0)}{\gamma} = \frac{1}{\gamma N_{sam}} \sum_{s=1}^{N_{sam}} \delta_0^{b^{(s)}} . \quad (40)$$

QED

4 Mean Values of Observables and Boltzmann Partition Function

In this section, we give algorithms for calculating, under various scenarios, the expected value of an observable Ω of a quantum system, and the Boltzmann partition function $Z = \sum_r e^{-\beta E_r}$ for an inverse temperature $\beta \in \mathbb{R}^{\geq 0}$, where E_r are the eigenvalues of the Hamiltonian of the quantum system.

Consider a quantum system with density matrix ρ and Hamiltonian H , where both operators act on \mathbb{C}^{N_S} . (careful: H is also used for the single qubit Hadamard transformation). Let

$$H | \hat{H} = E_x \rangle = E_x | \hat{H} = E_x \rangle \quad (41)$$

for $x \in Bool^{N_B}$. Define the basis-changer unitary operator U_H by

$$\langle y | U_H | x \rangle = \langle y | \hat{H} = E_x \rangle \quad (42)$$

for $x, y \in \text{Bool}^{N_B}$. Furthermore, consider a Hermitian operator Ω acting on \mathbb{C}^{N_S} (what we call an “observable” of the quantum system) with

$$\Omega|\hat{\Omega} = \Omega_x\rangle = \Omega_x|\hat{\Omega} = \Omega_x\rangle \quad (43)$$

and

$$\langle y|U_\Omega|x\rangle = \langle y|\hat{\Omega} = \Omega_x\rangle \quad (44)$$

for $x, y \in \text{Bool}^{N_B}$.

Some important scenarios that we would like to consider are

- (a) *Assume that Ω_x for all $x \in \text{Bool}^{N_B}$ and U_Ω are known. Furthermore, assume that we know how to p-compile U_Ω and $e^{i\rho\Delta t}$ for any $\Delta t \geq 0$. Then $\text{tr}(\Omega\rho)$ can be calculated as follows.*

In Claim 1, set $V = U_\Omega$, $A = \rho$ and $f(\xi) = \xi$ for $\xi \in \mathbb{R}^{\geq 0}$. Thus

$$\mu(x) = \langle x|U_\Omega^\dagger \rho U_\Omega|x\rangle \quad (45)$$

can be calculated p-efficiently for any $x \in \text{Bool}^{N_B}$. Now a quantum sampling algorithm like the quantum Gibbs sampling algorithm of Ref.[2] can be used to sample the probability distribution $P_{\underline{x}}(x) = \mu(x)$ given by Eq.(45). If this yields the sample points $x^{(s)}$ for $s = 1, 2, \dots, N_{\text{sam}}$, then

$$\text{tr}(\Omega\rho) \approx \frac{1}{N_{\text{sam}}} \sum_{s=1}^{N_{\text{sam}}} \Omega_{x^{(s)}}. \quad (46)$$

- (b) *Assume that Ω_x for all $x \in \text{Bool}^{N_B}$ and U_Ω are known. Furthermore, assume that we know how to p-compile U_Ω and $e^{iH\Delta t}$ for any $\Delta t \geq 0$. Let $\rho = \frac{e^{-\beta H}}{Z}$ where $\beta \in \mathbb{R}^{\geq 0}$ and $Z = \text{tr}(e^{-\beta H})$. Then $\text{tr}(\Omega\rho)$ can be calculated as follows.*

In Claim 1, set $V = U_\Omega$, $A = H$ and $f(\xi) = e^{-\beta\xi}$ for $\xi \in \mathbb{R}^{\geq 0}$. (Assume that the eigenvalues of H are bounded below, as is true for any physical Hamiltonian, and, if necessary, add a constant to H so as to make all its eigenvalues non-negative.) Thus

$$\mu(x) = \langle x|U_\Omega^\dagger e^{-\beta H} U_\Omega|x\rangle \quad (47)$$

can be calculated p-efficiently for any $x \in \text{Bool}^{N_B}$. Now a quantum sampling algorithm like the quantum Gibbs sampling algorithm of Ref.[2] can be used to sample $\mu(x)$ given by Eq.(47). (No need to know $\sum_x \mu(x)$ since the sampling algorithm only uses probability ratios.) If this yields the sample points $x^{(s)}$ for $s = 1, 2, \dots, N_{\text{sam}}$, then an estimate of the expected value of Ω is again given by Eq.(46).

- (c) Assume that function $g : \mathbb{R}^{\geq 0} \rightarrow \mathbb{R}^{\geq 0}$ is simple (that is, that it can be calculated p-efficiently). Assume that we know how to p-compile $e^{iH\Delta t}$ for any $\Delta t \geq 0$. Let $\rho = \frac{e^{-\beta H}}{Z}$ where $\beta \in \mathbb{R}^{\geq 0}$ and $Z = \text{tr}(e^{-\beta H})$. Let $Z_g = \text{tr}\{g(H)e^{-\beta H}\}$. Then Z_g and $\text{tr}\{g(H)\rho\}$ can be calculated as follows.

In Claim 1, set $V = 1$, $A = H$ and $f(\xi) = g(\xi)e^{-\beta\xi}$ for $\xi \in \mathbb{R}^{\geq 0}$. (If necessary, add a constant to H so as to make all its eigenvalues non-negative.) Thus

$$\mu(x) = \langle x | g(H) e^{-\beta H} | x \rangle \quad (48)$$

can be calculated p-efficiently for any $x \in \text{Bool}^{N_B}$. Now a quantum sampling algorithm like the quantum Gibbs sampling algorithm of Ref.[2] can be used to sample $\mu(x)$ given by Eq.(48). If this yields the sample points $x^{(s)}$ for $s = 1, 2, \dots, N_{sam}$, then an estimate \check{Z}_g of Z_g can be obtained as follows.

$$\check{P}_{\underline{x}}(x) = \frac{1}{N_{sam}} \sum_{s=1}^{N_{sam}} \delta_x^{x^{(s)}} \approx \frac{\mu(x)}{Z_g}, \quad (49)$$

$$\check{Z}_g = \frac{1}{N_{sam}} \sum_{s=1}^{N_{sam}} \frac{\mu(x^{(s)})}{\check{P}_{\underline{x}}(x^{(s)})} \approx Z_g. \quad (50)$$

To estimate $\text{tr}\{g(H)\rho\}$, we can use

$$\frac{\check{Z}_g}{\check{Z}_1} \approx \frac{Z_g}{Z_1} = \text{tr}\{g(H)\rho\}. \quad (51)$$

Note that if $g : \mathbb{R}^{\geq 0} \rightarrow \mathbb{R}$ instead of $g : \mathbb{R}^{\geq 0} \rightarrow \mathbb{R}^{\geq 0}$, one can set $g = g_+ - g_-$ where $g_{\pm} \geq 0$. Then $Z_g = Z_{g_+} - Z_{g_-}$. So we can estimate Z_g by first estimating $Z_{g_{\pm}}$. Since we can estimate Z_g and Z_1 , we can estimate $\text{tr}\{g(H)\rho\}$ using Eq.(51).

5 Comparisons with the Joneses

In this section, we compare the algorithms of this paper with algorithms in earlier papers for calculating the same things (“our competition”). This paper has not addressed the problem of finding useful estimates and bounds for the convergence rate and error of its algorithms. Such analysis will hopefully be done in future papers by me or others more capable. Lacking this analysis, the comparisons in this section should be taken as incomplete and preliminary.

Suppose \mathcal{V} is a Hilbert space and ρ is a density matrix acting on \mathbb{C}^{N_S} . Any pure state $|\Psi\rangle \in \mathbb{C}^{N_S} \otimes \mathcal{V}$ such that $\text{tr}_{\mathcal{V}}(|\Psi\rangle\langle\Psi|) = \rho$ is called a purification of ρ .

Given a probability distribution $P_{\underline{x}}(x)$, where $x \in Z_{0, N_S-1}$, it is convenient to define a $|\sqrt{P_{\underline{x}}}\rangle$ state by

$$|\sqrt{P_{\underline{x}}}\rangle = \sum_{x=0}^{N_S-1} \sqrt{P_{\underline{x}}(x)} |x\rangle. \quad (52)$$

Note that in the algorithms (a), (b), (c), finding the needed diagonal matrix elements is p-efficient. So the rate determining step of these algorithms is the quantum sampling part, which is not p-efficient. However, if the quantum sampling is done using the algorithm of Ref.[2], then the sampling converges (to a given precision) in $\mathcal{O}(\frac{1}{\sqrt{\delta}})$ steps, where δ is the distance between the two largest eigenvalue magnitudes of the underlying Markov chain.

Note also that none of the algorithms (a), (b), (c) ever physically produces a Boltzmann quantum state (either $\rho = e^{-\beta H}/Z$ or a purification thereof). They do produce $|\sqrt{P_{\underline{x}}}\rangle$ states.

Ref.[3] by Wocjan et al. presents an algorithm for calculating the partition function of a quantum system with Hamiltonian H , but it requires that the eigenvalues of H be known a priori (as is the case when the system is classical). The more recent Ref.[4] by Poulin and Wocjan does not require that the eigenvalues of H be known a priori. However, the algorithm of Ref.[4] physically creates a sequence of Boltzmann quantum states (purifications of $\rho = e^{-\beta H}/Z$), each state characterized by a different inverse temperature, with the sequence of inverse temperatures increasing gradually, according to an “annealing schedule”, from 0 towards the target β . Algorithm (c) also calculates the partition function of a quantum system without assuming that the eigenvalues of H are known a priori. But algorithm (c) never produces physically any Boltzmann quantum state. Nor does it introduce error at every stage of an annealing schedule (all its calculations are done at the target β).

Ref.[5] by Temme et al. gives an algorithm that physically produces a Boltzmann quantum state $\rho = e^{-\beta H}/Z$. Instead of producing this ρ or a purification of it, algorithm (b) produces a $|\sqrt{P_{\underline{x}}}\rangle$ state. If one wants to use the algorithm of Temme et al. to get $\text{tr}(\Omega\rho)$, one still must assume the same things as (b) above (namely, that Ω_x for all x and U_Ω are known, and that we know how to p-compile U_Ω and $e^{iH\Delta t}$). If these assumptions are satisfied, one can use the algorithm of Temme et al. to produce $U_\Omega^\dagger \rho U_\Omega$ physically, and then measure $|x\rangle\langle x|$ on it. After obtaining N_{sam} samples of x , one can then use Eq.(46) to estimate $\text{tr}(\Omega\rho)$. Thus, the Temme et al. algorithm assumes the same things as (b) to estimate $\text{tr}(\Omega\rho)$. A big advantage of (b) over Temme et al. is that (b) converges in $\mathcal{O}(\frac{1}{\sqrt{\delta}})$ steps, whereas Temme et al. converges, just like classical algorithms, in $\mathcal{O}(\frac{1}{\delta})$ steps.

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